

On the second-neighbor correlator in 1D XXX quantum antiferromagnetic spin chain

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Abstract

We have calculated the energy per site for the ground state of antiferromagnetic quantum spin chain with variable range exchange $h(j-k) \propto \sinh^2 a \sinh^{-2} a(j-k)$ in the framework of the asymptotic Bethe ansatz. By expanding it in powers of e^{-2a} , we have confirmed the value of the second-neighbor correlator for the model with nearest-neighbor exchange obtained earlier in the atomic limit of the Hubbard chain.

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At present, there are two main approaches in investigations of spin correlations in the ground state of the quantum Heisenberg antiferromagnet. The first one is connected with analysis of the representations of quantum groups [1] and gives some universal prescription of calculation of various correlations via multiple contour integrals. Unfortunately, till now there are no possibilities to reduce these multiple integrals to known transcendents. The second approach consists in finding correlators in the form of Fredholm determinants [2]. However, within this approach there is still no way to analytic evaluation of these Fredholm determinants. Asymptotics of spin correlations at large distances between spins has been obtained in the framework of conformal field theory [3], but this theory cannot give the values of correlators at finite distances.

The first explicit calculation of nearest-neighbor spin correlator $\langle \vec{\sigma}_j \vec{\sigma}_{j+1} \rangle$ in the thermodynamic limit has been made by Hulthen [4] with the use of the Bethe ansatz [5]. Since this correlator coincides with the energy per site in the vacuum state of the model, the problem is equivalent to calculation of this energy for finite number of lattice sites N and taking thermodynamic limit $N \rightarrow \infty$. The second-neighbor correlator $\langle \vec{\sigma}_j \vec{\sigma}_{j+2} \rangle$ has been calculated by Takahashi [6] with the use of perturbation theory in the atomic limit of the half-filled Hubbard model. This result has never been confirmed by other scheme of calculations.

In this letter, we perform the explicit calculation of $\langle \vec{\sigma}_j \vec{\sigma}_{j+2} \rangle$ by using the way which differs substantially from the way of ref.[6]. Namely, we start from the consideration of the integrable spin chain with variable range exchange and the Hamiltonian [7]

$$\mathcal{H} = \frac{1}{2} \sum_{j \neq k} \frac{\sinh^2 a}{\sinh^2 a(j-k)} \frac{\vec{\sigma}_j \vec{\sigma}_k - 1}{2}. \quad (1)$$

In the nearest-neighbor limit $a \rightarrow \infty$ one can decompose (1) into a series

$$\mathcal{H} = \frac{1}{2} \sum_j (\vec{\sigma}_j \vec{\sigma}_{j+1} - 1) + \frac{1}{2} e^{-2a} \sum_j (\vec{\sigma}_j \vec{\sigma}_{j+2} - 1) + o(e^{-2a}). \quad (2)$$

Hence one can write the ground-state energy per site as

$$e = \frac{1}{2} \langle \vec{\sigma}_j \vec{\sigma}_{j+1} - 1 \rangle + \frac{1}{2} e^{-2a} \langle \vec{\sigma}_j \vec{\sigma}_{j+2} - 1 \rangle + o(e^{-2a}), \quad (3)$$

where $\langle \rangle$ means average on the vacuum state of the Hamiltonian (2). Fortunately, in

the first order approximation (3) one can replace this state to the vacuum state of nonperturbed Hamiltonian with the interaction of nearest-neighbor spins, $\mathcal{H}_0 = \frac{1}{2} \sum_j (\vec{\sigma}_j \vec{\sigma}_{j+1} - 1)$.

Let us now calculate the ground-state energy per site (3) of the model with the use of the asymptotic Bethe ansatz (ABA) [8]. The wave functions of the states with M down spins can be calculated exactly [7]. Their asymptotic expression in the region $n_1 \ll n_2 \dots \ll n_M$ has the form similar to Bethe one,

$$\psi(n_1, ..n_M) \propto \sum_{P \in \pi_M} \exp \left(i \sum_{\alpha=1}^M k_{P\alpha} n_\alpha \right) \exp \left(\frac{i}{2} \sum_{\alpha < \beta}^M \chi(k_{P\alpha}, k_{P\beta}) \right), \quad (4)$$

where the first sum is taken over all permutations from the group π_M , $\{k_\alpha\}$ is the set of pseudomomenta and $\chi(k_\alpha, k_\beta)$ is the two-magnon phase shift defined by the relations

$$\cot \frac{\chi(k_\alpha, k_\beta)}{2} = \varphi(k_\alpha) - \varphi(k_\beta), \quad (5)$$

$$\varphi(k) = \frac{k}{2\pi i a} \zeta_1 \left(\frac{i\pi}{2a} \right) - \frac{1}{2ia} \zeta_1 \left(\frac{ik}{2a} \right), \quad (6)$$

where ζ_1 is the zeta Weierstrass function defined on the torus $\mathbf{T}_1 = \mathbf{C}/(\mathbf{Z} + \frac{i\pi}{a}\mathbf{Z})$. To consider the chains of finite length N in the thermodynamic limit $N \rightarrow \infty$, we adopt the main hypothesis of ABA, i.e. imposing periodic boundary conditions on the asymptotic form of the wave function (4) (it is worth noting here that the exact solution of the problem of finite chains in the model should be based on the treatment of the Hamiltonian with the exchange given by the Weierstrass \wp function instead of (1), and is not available till now except the cases $M = 2, 3$). Taking $\psi(n_2, ..n_M, n_1 + N) = \psi(n_1, ..n_M)$ and calculating the both sides with the use of the formula (4) results in the ABA equations

$$\exp(ik_\alpha N) = \exp \left(i \sum_{\beta \neq \alpha}^M \chi(k_\alpha, k_\beta) \right), \quad \alpha = 1, ..M. \quad (7)$$

The energy of corresponding configuration is given by

$$E_M = \sum_{\alpha=1}^M \sum_{n \neq 0} \frac{\sinh^2 a}{\sinh^2 an} (\cos(k_\alpha n) - 1). \quad (8)$$

We are interested in the antiferromagnetic vacuum of the model and should take N even, $M = N/2$. Taking logarithms of both sides of (7) and choosing the proper branches [9], one arrives at

$$\frac{Q_\alpha}{N} = \frac{\pi - k_\alpha}{2\pi} - \frac{1}{\pi N} \sum_{\beta \neq \alpha}^M \arctan[\varphi(k_\alpha) - \varphi(k_\beta)]. \quad (9)$$

We adopt usual hypothesis about the distribution of the (half)integers $\{Q\}$ for antiferromagnetic vacuum state. Namely, it will be assumed that these numbers form uniform string from $-Q_{max}$ to Q_{max} , $Q_{max} = N/4 - 1/2$ without holes. We introduce the rapidity variable λ by the relation $\lambda = \varphi(k)$ and the function $\mu(\lambda)$ via the relation $\pi - k = \mu(\lambda)$. The ABA equations (9) now can be written as

$$Q_\alpha/N = Z(\lambda_\alpha), \quad (10)$$

where

$$Z(\lambda) = (2\pi)^{-1}\mu(\lambda) - \frac{1}{\pi N} \sum_{\beta=1}^{\infty} \arctan(\lambda - \lambda_\beta).$$

Following Hulthen [4], let us go to continuous variable $x = Q_\alpha/N$ in the limit $N \rightarrow \infty$ and introduce the root density $\sigma_N(\lambda)$ by the relation $\sigma_N(\lambda) = dx/d\lambda$. Differentiating both sides of (10) with respect to λ , one arrives at the Hulthen-like equation in the limit $N \rightarrow \infty$

$$\sigma_\infty(\lambda) = (2\pi)^{-1}\mu'(\lambda) - \int_{-\infty}^{\infty} A(\lambda - \lambda')\sigma_\infty(\lambda')d\lambda', \quad (11)$$

where $A(\lambda) = [\pi(1 + \lambda^2)]^{-1}$. The energy per site can be written from (8) as

$$e_\infty = \lim_{N \rightarrow \infty} N^{-1}E_{N/2} = \int_{-\infty}^{\infty} \varepsilon(k(\lambda))\sigma_\infty(\lambda)d\lambda, \quad (12)$$

where

$$\varepsilon(k(\lambda)) = 2 \sinh^2 a \sum_{n=1}^{\infty} \frac{\cos nk(\lambda) - 1}{\sinh^2 an}. \quad (13)$$

The solution to (11) can be found via Fourier transform,

$$\sigma_\infty(\lambda) = (2\pi)^{-2} \int_{-\infty}^{\infty} \frac{e^{i\lambda p} dp}{1 + e^{-|p|}} \int_{-\infty}^{\infty} \mu'(\tau) e^{-ip\tau} d\tau.$$

Substituting it into (12) yields

$$e_\infty = (2\pi)^{-2} \int_{-\infty}^{\infty} d\lambda \varepsilon(k(\lambda)) \int_{-\infty}^{\infty} dp \frac{e^{ip\lambda}}{1 + e^{-|p|}} \int_{-\infty}^{\infty} \mu'(\tau) e^{-ip\tau} d\tau.$$

Choosing variables as $\lambda = \varphi(k)$, $\mu'(\tau)d\tau = -dk'$ and changing the order of integration (it is allowed since the integral over τ vanishes sufficiently fast as $|p| \rightarrow \infty$), one arrives at the main formula

$$e_\infty = -(2\pi)^{-2} \int_{-\infty}^{\infty} \frac{dp}{1 + e^{-|p|}} \int_0^{2\pi} dk \varepsilon(k) \varphi'(k) e^{ip\varphi(k)} \int_0^{2\pi} dk' e^{-ip\varphi(k')}, \quad (14)$$

where the functions $\varepsilon(k)$ and $\varphi(k)$ are determined by (13) and (6). The integrals in (14) cannot be calculated analytically. However, one can see from (6) and (13) that for large a

$$\varphi(k) = \frac{1}{2} \cot \frac{k}{2} + 2e^{-2a} \sin k + o(e^{-2a}), \quad (15)$$

$$\varepsilon(k) = 2(\cos k - 1) + 2e^{-2a}(\cos 2k - 1) + o(e^{-2a}). \quad (16)$$

Substituting (15) and (16) into (14), one can calculate inner integrals up to the order of e^{-2a} ,

$$\begin{aligned} \int_0^{2\pi} dk' e^{-ip\varphi(k')} &= 2\pi(1 - p^2 e^{-2a})e^{-|p/2|} + o(e^{-2a}), \\ \int_0^{2\pi} dk \varepsilon(k) \varphi'(k) e^{ip\varphi(k)} &= \pi(2 + e^{-2a}(8 - p^2))e^{-|p/2|} + o(e^{-2a}). \end{aligned}$$

Now, taking into account the formula $\int_0^\infty \frac{p^2 dp}{1+e^p} = 3/2\zeta(3)$, where ζ is the Riemann zeta function, the two leading terms of e_∞ are calculated. The comparison of (3) and (14) then gives

$$\langle \vec{\sigma}_j \vec{\sigma}_{j+2} \rangle = 1 - 16 \ln 2 + 9\zeta(3), \quad (17)$$

which coincides exactly with the expression given by Takahashi [6].

To conclude, we would like to point out that our approach to the calculation of the correlator is based on the hypothesis of the validity of the ABA and uniform distribution of the numbers Q_α for the antiferromagnetic vacuum of the model (1). The approach of ref.[6] refers to the perturbation theory in the atomic limit of half-filled Hubbard model and the integral representation of its ground-state energy in the thermodynamic limit which is derived under the assumption on uniform distribution of integers in the Bethe ansatz equations for the model. Hence both results are not absolutely rigorous from mathematical point of view, and their coincidence supports the validity of both approaches. Unfortunately, neither our method nor the method of Takahashi [6] can be used for the calculations of higher correlators. It seems that these calculations will be possible if one will find the method of reduction of multiple integrals in general formulae of [4]. Till now, there is no recipe of doing this even for the second-neighbor correlator (17).

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